

REPORT DOCUMENTATION PAGE			Form Approved OMB NO. 0704-0188		
<p>The public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA, 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.</p> <p>PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.</p>					
1. REPORT DATE (DD-MM-YYYY) 08-07-2016		2. REPORT TYPE Final Report		3. DATES COVERED (From - To) 1-May-2013 - 30-Apr-2016	
4. TITLE AND SUBTITLE Final Report: Quantum Engineering of Dynamical Gauge Fields on Optical Lattices			5a. CONTRACT NUMBER W911NF-13-1-0119		
			5b. GRANT NUMBER		
			5c. PROGRAM ELEMENT NUMBER 206022		
6. AUTHORS Shan-Wen Tsai, Yannick Meurice			5d. PROJECT NUMBER		
			5e. TASK NUMBER		
			5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAMES AND ADDRESSES University of California - Riverside 200 University Office Building Riverside, CA 92521 -0001			8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211			10. SPONSOR/MONITOR'S ACRONYM(S) ARO		
			11. SPONSOR/MONITOR'S REPORT NUMBER(S) 62897-PH-REP.15		
12. DISTRIBUTION AVAILABILITY STATEMENT Approved for Public Release; Distribution Unlimited					
13. SUPPLEMENTARY NOTES The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.					
14. ABSTRACT In this project, we have developed a scheme for using cold atom systems on optical lattices as quantum simulators for lattice gauge theories. We designed cold atom experimental setups that could be used to learn about the phase diagrams of Lattice Gauge Theory models and real time evolution, which cannot be studied using conventional methods. We first constructed a sequence of theoretical steps connecting the classical O(2) model in 1+1 dimensions to a boson model that can be implemented on optical lattices, showing a proof of principle that quantum computing via					
15. SUBJECT TERMS quantum simulation, lattice gauge theory, optical lattices, cold atoms					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Shan-Wen Tsai
a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU			19b. TELEPHONE NUMBER 951-827-1057

Report Title

Final Report: Quantum Engineering of Dynamical Gauge Fields on Optical Lattices

ABSTRACT

In this project, we have developed a scheme for using cold atom systems on optical lattices as quantum simulators for lattice gauge theories. We designed cold atom experimental setups that could be used to learn about the phase diagrams of Lattice Gauge Theory models and real time evolution, which cannot be studied using conventional methods.

We first constructed a sequence of theoretical steps connecting the classical $O(2)$ model in 1+1 dimensions to a boson model that can be implemented on optical lattices, showing a proof-of-principle that quantum computing via optical lattices is possible for classical lattice models. We then extended this protocol to limits of the Abelian Higgs model, a model that exhibits important features of QCD such as confinement. Our results include construction of effective actions, testing with Monte Carlo simulations, tensor renormalization group technique development and application, mappings to quantum spin and boson Hamiltonians, and analysis of candidate systems for experimental realization. We verified that in the superfluid phase the central charge can be extracted from the entanglement entropy as predicted by conformal symmetry. We calculated and compared the Polyakov loop, an order parameter for confinement, in the two formulations, and propose that it can be a useful quantity to probe experimentally. The results from our project opens the door for exciting new research directions, such as quantum simulation of the Schwinger model and of non-Abelian models.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
08/29/2014	3.00 Chen-Yen Lai, Wen-Min Huang, David K. Campbell, Shan-Wen Tsai. $\langle \mathbf{x} \cdot \mathbf{y} \rangle$ -density wave in fermion-fermion cold-atom mixtures, Physical Review A, (07 2014): 13610. doi: 10.1103/PhysRevA.90.013610
08/31/2015	5.00 Yuzhi Liu, Chen-Yen Lai, J. Unmuth-Yockey, Li-Ping Yang, A. Bazavov, Z. Y. Xie, T. Xiang, S. Chandrasekharan, Haiyuan Zou, S.-W. Tsai, Y. Meurice. Progress towards quantum simulating the classical $O(2)$ Model, Physical Review A, (12 2014): 1. doi: 10.1103/PhysRevA.90.063603
TOTAL:	2

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
-----------------	--------------

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

- 1) "Toward quantum chromodynamics calculations with optical lattices", invited seminar by Yannick Meurice, Hamburg University, Hamburg, Germany, August 2013.
- 2) "Toward quantum chromodynamics calculations with optical lattices", invited seminar by Yannick Meurice, Utrecht University, Utrecht, Netherlands, August 2013.
- 3) "From classical computing to quantum simulators: a tensor renormalization group approach", seminar by Yannick Meurice, University of Heidelberg, Heidelberg, Germany, February 17, 2014.
- 4) "Taming sign problems using tensor renormalization", oral presentation by Yannick Meurice, EMMI Workshop: SIGN 2014 International Workshop on the Sign Problem in QCD and Beyond, Darmstadt, Germany, February 18-21, 2014.
- 5) "Improving the Hubbard-Lattice Gauge Theory correspondence on optical lattices", Yannick Meurice, Alexei Bazavov, Yuzhi Liu, Chen-Yen Lai, Shan-Wen Tsai, contributed talk, American Physical Society March Meeting, Denver, CO, USA, March 3-7, 2014.
- 6) " d_{xy} -density wave in fermion-fermion cold atom mixtures", Chen-Yen Lai, Wen-Min Huang, David K. Campbell, Shan-Wen Tsai, contributed talk, American Physical Society March Meeting, Denver, CO, USA, March 3-7, 2014.
- 7) "Towards quantum computing for the classical $O(2)$ model", presented by Yannick Meurice, Nuclear/Particle Physics Seminar, University of Colorado, Boulder, CO, USA, March 4, 2014.
- 8) "Towards quantum computing for the classical $O(2)$ model", seminar by Yannick Meurice, Laboratoire de Physique Théorique de la Matière Condensée, Université Pierre et Marie Curie, Place Jussieu, Paris, France, March 24, 2014.
- 9) "Towards quantum computing for the classical $O(2)$ model", seminar by Yannick Meurice, Institut de Physique Théorique, CEA Saclay, Gif-sur-Yvette, France, March 27, 2014.
- 10) "Towards Implementations of Lattice Gauge Theories on Optical Lattices", oral presentation by Yannick Meurice, KITPC Program "Precision Many-body Physics of Strongly correlated Quantum Matter", KITPC, Beijing, China, May 5-June 13, 2014.
- 11) "Numerical Methods for Lattice Gauge Theories: Basic Ideas and New Developments", oral presentation by Yannick Meurice, KITPC Summer School on Advanced Numeric Methods of Quantum Statistics, KITPC, Beijing, China, May 26-30, 2014.
- 12) "The effective $U(1)$ -Higgs theory at strong coupling on optical lattices?", poster presentation by Alexei Bazavov, Lattice 2014, The 32nd International Symposium on Lattice Field Theory (LATTICE 2014), Columbia University, New York, June 23-28, 2014.
- 13) "Ultracold Atoms and New Routes to Quantum Simulations", lecture for high school physics teachers by Shan-Wen Tsai, 2014 Summer Physics Teacher Academy, Department of Physics and Astronomy, University of California, Riverside, June 23-27, 2014
- 14) "Tensor Renormalization Group approach of lattice models: from exact blocking formulas to accurate numerical results", Li-Ping Yang, Yuzhi Liu, Haiyuan Zou, Z. Y. Xie, and Y. Meurice (presenter), Conference on the Exact Renormalization Group 2014, Lefkada, Greece, September 26, 2014.
- 15) "Improving the Hubbard-Lattice Gauge Theory correspondence on optical lattices", Y. Meurice, University of Iowa, IA, USA, February 23, 2015.
- 16) "The Abelian Higgs model on Optical Lattices?", Y. Meurice (presenter), S.-W. Tsai, A. Bazavov, and J. Zhang, APS March Meeting, San Antonio, TX, USA, March 2-6, 2015.
- 17) "Gauge Invariant Implementation of the Abelian Higgs model on Optical Lattices", seminar by Y. Meurice, INT Program Frontiers in Quantum Simulation with Cold Atoms, Institute for Nuclear Theory, University of Washington, Seattle, WA, USA, March 23 - May 8, 2015.
- 18) "Gauge Invariant Implementation of the Abelian Higgs model on Optical Lattice", poster presentation by Y. Meurice, Conference on Frontiers in Quantum Simulation with Cold Atoms, Institute for Nuclear Theory, U. of Washington, Seattle, WA, USA, March 30 - April 2, 2015.
- 19) "Entanglement entropy of the $O(2)$ model", informal presentation by Y. Meurice, Aspen Center for Physics, Aspen, CO, USA, June 2, 2015.
- 20) "Gauge-invariant implementation of $U(1)$ -Higgs model on optical lattices", seminar by A. Bazavov, Institute of Photonic Sciences, Barcelona, Spain, June 19, 2015.

- 21) "The Tensor Renormalization Group approach of lattice models: from exact blocking formulas to accurate numerical results", oral presentation by Y. Meurice, The 33 International Symposium on Lattice Field Theory (Lattice 2015), Kobe, Japan, July 14-18, 2015.
- 22) "Effective action for the Abelian Higgs model for a gauge-invariant implementation on optical lattices", oral presentation by A. Bazavov, The 33 International Symposium on Lattice Field Theory (Lattice 2015), Kobe, Japan, July 14-18, 2015.
- 23) "D-wave density waves in fermionic mixtures", oral presentation by S.-W. Tsai, Workshop Ultra-Cold Quantum Matter with Atoms and Molecules, Aspen Center for Physics, Aspen, CO, USA, July 15, 2015.
- 24) "Proposals for quantum simulating simple lattice gauge theory models using optical lattices" Jin Zhang, Judah Unmuth-Yockey, Alexei Bazavov, Yannick Meurice, Shan-Wen Tsai, APS March Meeting, Baltimore, MD, USA, March 14-18, 2016.
- 25) "Matrix Product States" Karl Jansen (moderator), Mari Carmen Bañuls, Ignacio Cirac, Yannick Meurice, Roundtable Discussion, Symposium on Effective Field Theories and Lattice Gauge Theory, Institute for Advanced Study, Technical University of Munich, Munich, Germany, May 18-21, 2016.
- 26) "Proposals to implement the Abelian Higgs model on optical lattices", invited seminar by Yannick Meurice, Max-Planck-Institut für Quantenoptik, Munich, Germany, May 24, 2016.
- 27) "Classical and Quantum Computing near Conformality", Yannick Meurice, Conference on Emergent Properties of Space-Time, CERN, Geneva, Switzerland, June 20 - July 1, 2016.

Number of Presentations: 27.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

<u>Received</u>	<u>Paper</u>
06/28/2016 6.00	Alexei Bazavov, Chen-Yen Lai, Shan-Wen Tsai, Yannick Meurice. The effective U(1)-Higgs theory at strong couplings on optical lattices?, Lattice 2014 - The 32nd International Symposium on Lattice Field Theory. 23-JUN-14, Columbia University, New York, NY, USA. : ,
06/30/2016 12.00	. Effective action for the Abelian-Higgs model for a gauge-invariant implementation on optical lattices, The 33rd International Symposium on Lattice Field Theory. 14-JUL-15, Kobe, Japan. : ,
06/30/2016 13.00	. Approaching conformality with the Tensor Renormalization Group method, The 33rd International Symposium on Lattice Field Theory. 14-JUL-15, Kobe, Japan. : ,
07/06/2016 14.00	. The effective U(1)-Higgs theory at strong coupling on optical lattices?, 32nd International Symposium on Lattice Field Theory. 23-JUN-14, Columbia University, New York, NY, USA. : ,
TOTAL:	4

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received

Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	Discipline
Chen-Yen Lai	0.09	
Jin Zhang	0.18	
FTE Equivalent:	0.27	
Total Number:	2	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Alexei (Oleksiy) Bazavov	1.00
FTE Equivalent:	1.00
Total Number:	1

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Shan-Wen Tsai	0.07	
Yannick Meurice	0.07	
FTE Equivalent:	0.14	
Total Number:	2	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME

Jin Zhang

Total Number: 1

Names of personnel receiving PHDs

NAME

Chen-Yen Lai

Total Number: 1

Names of other research staff

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

(1) Foreword

This is the Final Progress Report for the project “Quantum Engineering of Dynamical Gauge Fields on Optical Lattices”, Proposal Number 62897PHREP, Funding Number W911NF1310119, with Prof. Shan-Wen Tsai from University of California Riverside and Prof. Yannick Meurice from University of Iowa as Principal Investigators.

This project has developed a scheme for using cold atoms on optical lattices to mimic simulations performed in Lattice Gauge Theory (LGT), designing experimental setups that could be used to quantum-simulate Lattice Gauge Theory models, including their phase diagrams and real time evolution, which cannot be studied using currently available conventional methods based on importance sampling (Monte Carlo simulations).

(2) Statement of the problem studied

Dynamical gauge fields are essential to produce the short and large distance behavior of gauge theories, which have been exploited very successfully in particle physics. With the remarkable developments in the field of cold atoms, models such as ones studied in Condensed Matter Physics for their relevance to complex materials may be engineered and tested. The problem that we tackled in this project was to find ways in which the rapidly evolving technology of cold atoms on optical lattices can be used to mimic simulations performed in LGT. The goal was to design experimental setups that can be used as table-top quantum simulators for the phase diagrams of LGT models and their real time evolution, aspects that cannot be studied using conventional, Monte-Carlo-based, simulation methods (classical computing) that are currently available. Below we describe the results we obtained under this goal. In this project we also explored connections between LGT and Hubbard-like models studied in Condensed Matter Physics.

(3) Summary of the most important results

We first constructed a sequence of theoretical steps connecting the classical $O(2)$ model in 1+1 dimensions (one space and one Euclidean time dimensions) to physical models that can potentially be implemented with cold atoms or molecules on optical lattices, and evolving in physical time, showing a proof of principle, through this simple example, that quantum computing via optical lattices is possible for classical lattice models. These results were published in a Physical Review A article[1] and in various conferences and seminars.

In the literature, the classical $O(2)$ model is sometimes called the classical XY model.

We then extended this protocol to limits of the Abelian Higgs model (scalar electrodynamics) in 1+1 dimensions. This is a gauged version of the $O(2)$ model discussed above. The significance is that, with this achievement, we now have a proposal for an experimental implementation that can quantum simulate a LGT model that exhibits important features of Quantum Chromodynamics (QCD), such as confinement. We constructed a gauge-invariant effective action by integrating out the gauge field and expanding in the hopping parameter, testing it with Monte Carlo simulations for small values of the self-coupling. For infinitely large self-coupling, the Higgs mode is frozen, the partition function can be written in terms of local tensors and we applied the Tensor Renormalization Group (TRG) method to calculate the spectrum and take the time continuum limit numerically. At zero gauge coupling and with a spin-1 truncation, the small volume energy spectrum is identical to the low energy spectrum of a two-species Bose-Hubbard model at strong coupling. We extended the procedure to finite gauge couplings, deriving a spin-1 approximation of the Hamiltonian and proposing realistic optical lattice implementations. These results were published in Physical Review D [2]. Some of these results have also been presented in conferences and in seminars at various institutions as well as in a conference proceedings papers [3,4].

Additionally, we studied the fine structure of the entanglement entropy in the classical $O(2)$ model [5,6]. Recent progress in the experimental manipulation of cold atoms has made possible detailed study of the entanglement entropy of small systems. It is important to be able to calculate theoretically the entanglement entropy for the models that we propose to quantum simulate. For this purpose we have developed methods based on the TRG (described in more detail below in Subsection (3a)).

We have compared two calculations of the particle density in the superfluid phase of the classical $O(2)$ model with a chemical potential in 1+1 dimensions. The first relies on exact blocking formulas from the TRG formulation of the transfer matrix. The second is a worm algorithm. The particle number distributions obtained with the two methods agree well. We used the TRG method to calculate the thermal entropy and the entanglement entropy. We described the particle density, the two entropies and the topology of the world lines as we increased the chemical potential to go across the superfluid phase between the first two Mott insulating phases. For a sufficiently large temporal size, this process reveals an interesting fine structure: the average particle number and the winding number of most of the world lines in the Euclidean time direction increase by one unit at a time. At each step, the thermal entropy develops a peak and the entanglement entropy increases until we reach half-filling and then decreases in a way that approximately mirrors the ascent, a fact that can be explained by an approximate particle-hole symmetry.

We have also developed a computer code suite for simulating the Abelian and non-Abelian gauge-Higgs systems, as described in more detail in Subsection (3b).

We have verified that in the superfluid phase the central charge can be extracted from the entanglement entropy as predicted by conformal symmetry. We calculated and compared the Polyakov loop, an order parameter for confinement, in the Lagrangian and Hamiltonian formulations, and proposed that it can be a useful quantity to probe experimentally. More details on the effective quantum Hamiltonians and possible experimental realizations is provided in Subsection (3c). More details on using the entanglement entropy and the Polyakov loop to probe the phase diagram are provided in Subsection (3d). A preprint reporting these results is in progress.

This project supported work by one postdoc, Dr. Alexei Bazavov, and two graduate students, Dr. Chen-Yen Lai (04/2013 – 06/2014), who obtained his PhD in June 2014, and Mr. Jin Zhang (07/2014 – 04/2016), who is working towards his PhD degree at the University of California Riverside. We mentored two high school students (Mr. Jens Dancer and Ms. Sonali Durham, Iowa City High School, Iowa City, IA) and two undergraduate students (Mr. Keshav Suttrave and Mr. Zhuohao Liu, at University of Iowa). A grant from the High School Apprenticeship Program (HSAP)/Undergraduate Research Apprenticeship Program (URAP) of the Army Education Outreach Program provided financial support for one high school student and one undergraduate student.

(3a) Tensor renormalization-group formulation and results

The Tensor Renormalization Group (TRG) is a recently developed method [7]. It can be used to perform the strong coupling expansion, calculate critical exponents [8] and deal with the sign problem [9] preventing direct classical and quantum Monte Carlo simulations. This method can be applied to most models studied by lattice gauge theorists. The TRG method combined with a higher-order singular value decomposition (HOTRG) has been used to calculate the complex partition functions of the two-dimensional (2D) classical Ising and $O(2)$ (also called XY) models with complex beta [9] and with a chemical potential [1]. It has been used to calculate the phase diagram of the $O(2)$ model with a chemical potential.

We have been optimizing and improving Higher Order Tensor Renormalization Group (HOTRG) code for the Tensor Renormalization Group by exploiting its symmetries. We specifically used the charge conservation inherent in the two-dimensional $O(2)$ spin model to create a sparse HOTRG code [4]. The code cuts down CPU time by at least a magnitude of ten, if not more. It also scales considerably better than the original HOTRG code with the number of states kept during truncation.

The TRG method allowed us to reformulate the Abelian Higgs model exactly in terms of gauge invariant variables which were used directly in the quantum simulator proposal of Ref. [2].

(3b) Code development

Our project has demonstrated that properly designed LGT models behave approximately like many body systems in situations where numerical simulations are possible for both types of models. For this, it is thus important that we developed generic LGT codes that can be used in many different situations. Various codes were developed in our project by Dr. Bazavov and included in a code suite. It is based on the SciDAC [10] software developed by the Lattice QCD community for calculations in QCD [11]. In particular, the SciDAC software consists of five layers of libraries, QMP, QIO, QLA, QDP and QOPQDP, that provide fully parallelized routines for major computational operations needed in QCD. Dr. Bazavov took advantage of this existing high-level optimized software, and has added the routines for $U(1)$ pure gauge theory, complex scalar field theory, and the gauge version of the latter, i.e. scalar QED (sometimes also called the Abelian Higgs model).

We first focused on scalar QED and established the correspondence to the Bose-Hubbard model. In particular, we considered scalar QED at strong coupling. In this case, at the lowest order, the gauge part of the action can be neglected and then the integration on the gauge fields can be performed exactly. This generates a series in powers of products of four scalar fields. Thus, at the lowest order, it resembles the structure of the Bose-Hubbard model. This way, we were able to test the range of applicability of the strong-coupling expansion, by doing Monte Carlo simulations of the scalar QED.

The codes developed by Dr. Bazavov in this project allow for anisotropy between spatial and temporal couplings. This allows one to control the time continuum limit and connect smoothly from the Lagrangian to Hamiltonian formulation of the theory. This is important for our project, because the lattice QCD calculations are almost exclusively done in the Lagrangian formalism, while evolution on the optical lattices is naturally Hamiltonian. The Hubbard-type models to which we finally established a correspondence to are also normally formulated and solved in the Hamiltonian formalism.

The next stage in the development of our code suite consisted of simulating Abelian gauge-Higgs systems. In our recent publication [2] we simulated the Abelian-Higgs model and found very good agreement with the existing strong coupling

expansions [13]. For efficient simulation of the scalar field we rely on the algorithm of Ref. [14], which has high acceptance rate in the region of small self-coupling. This is the most explored region on the lattice, for the studies of the Abelian-Higgs model in the context of the electro-weak physics. We, however, need to be able to simulate the model for any value of the self-coupling. In particular, for the mapping of the Abelian-Higgs model to the two-species Bose-Hubbard model in Ref. [2], we considered the case of infinite self-coupling (which corresponds to frozen radial, or Higgs, mode of the scalar field).

For arbitrary self-coupling, local updating Monte Carlo algorithms are inefficient, since the quartic term (often called a “phi-four” interaction) can no longer be considered as a perturbation. The solution for this, that we pursued, is along the lines of Biased Metropolis-Heatbath Algorithm (BMHA) (Ref. [14], co-authored by Dr. Bazavov). In this case, the proposal probability is approximated by a piece-wise linear function, which is then tabulated and a new value for the random variable is generated from table lookups. Originally, BMHA has been developed for compact variables, and we extended it for noncompact case, such as the amplitude of the scalar field.

We developed a scalar version of the code for testing and small-scale simulation purposes. The machinery will be incorporated into the SciDAC libraries based fully parallel software [10].

Current code incorporates in a uniform fashion the “phi-four”-theory for real, complex and complex doublet fields and their gauged versions with $U(1)$ and $SU(2)$ gauge groups.

In Ref. [2] we have derived an effective gauge-invariant action which also includes quartic interactions, so BMHA is also a good choice for simulating that model.

For simulations we used facilities at the Fermi National Laboratory provided under a type C proposal to the USQCD lattice collaboration [15].

3c- Bose-Hubbard model and potential experimental realization with cold atoms

We first derived a quantum Hamiltonian that can be used to simulate the $O(2)$ model [1], and then proposed a gauge-invariant implementation of the $U(1)$ -Higgs model on optical lattices [2]. In both cases, the effective quantum Hamiltonian is a generalized Bose-Hubbard model with two species of bosons at strong coupling and special relations between the various interactions and the hopping parameter, that can be realized with cold atoms or molecules on optical lattices.

The effective quantum Hamiltonian for the case of the $O(2)$ model is a two-species Bose Hubbard model that at strong coupling, up to second order in degenerate perturbation theory, corresponds to the spin-1 projection of the rotor Hamiltonian [1]. This two-species Bose-

Hubbard model can be realized in a Rubidium-87 and Potassium-41 Bose-Bose mixture where an interspecies Feshbach resonance is accessible. A small repulsion between atoms in nearest-neighbor sites is also required. A few proposals may be explored on how to create such a term in cold atom systems on optical lattices, such as using dipolar bosons, by pumping bosons to higher Bloch bands, or via mediated interactions in multicomponent mixtures. We studied a $SU(2) \times SU(2)$ fermion-fermion mixture on a square lattice and have found a robust mechanism for creating unconventional density-wave states (with d-wave symmetry) when the two fermion have imbalanced populations near half-filling [16]. In this state, there is density wave modulations on alternating bonds due to an effective long-range attractive intra-species interaction generated by the other species. A similar mechanism, namely effective long-range interaction mediated by other species may also be explored in engineering the required Bose Hubbard terms for the quantum simulator.

For the Abelian Higgs model, an on-site term that converts bosons of one species into another species is needed [2]. This requirement rules out implementing this Hamiltonian using mixtures of two different types of atoms such as a mixture of Rubidium-87 and Potassium-41, which we proposed for the $O(2)$ model. It would be possible, however to implement it using a mixture of atoms in two hyperfine states that support Raman transitions between them. Another candidate system would be to use a single atomic species on a ladder structure with the two species indices corresponding to the atoms sitting in one or the other leg of the ladder. In this case, conversion between species would correspond to hopping along the rungs of the ladder.

(3d) Phase Diagram Probed by the Entanglement Entropy and the Polyakov Loop

The phase diagram of the $O(2)$ model is separated into Mott insulator phases with integer number of particles per site and a superfluid phase where the density increases with the chemical potential. In the superfluid phase, one expects that the model exhibits conformal symmetry at infinite volume with a central charge $c = 1$, which corresponds to a massless scalar field. At finite volume, this is signaled by an increase of the entanglement entropy with the size of the system L at a rate $(c/3) \cdot \ln(L)$ for periodic boundary conditions and $(c/6) \cdot \ln(L)$ for open boundary conditions[17]. We were able to verify this expectation using the TRG method (described above) and the corresponding Density Matrix Renormalization Group (DMRG) method for L up to 32. For larger L , the results were slightly below the linear behavior (Cardy scaling) but sensitive to the truncation dimension and by increasing this dimension, we observed that the results were getting closer to the expected Cardy scaling. Extrapolation procedures are being designed for sizes comparable to existing optical lattices (100-200 sites in typical experiments). Improved

methods of calculations based on the Multi-Scale Entanglement Renormalization Ansatz (MERA) idea are being designed.

Entanglement entropy is a quantity being actively studied in many diverse fields of physics as it contains information about non-local correlations in quantum systems and is key for quantum information. These fields include High Energy Physics, Cold Atom Physics, Condensed Matter Physics, and Quantum Gravity. Much effort has been put in developing experimental techniques to directly measure the entanglement entropy in cold atom systems [18,19]. In Ref. [18], the authors directly measure the Renyi entanglement entropy by preparing two identical copies of a many-body state and interfering them. Our results show that different quantum phases can be identified by the behavior of the entanglement entropy across the phase transition. Furthermore, finite size scaling can allow experimental measurement of universal quantities such as the central charge c . Our numerics show that c can be obtained even for relatively small ranges of the system size L .

In our reformulation of the Abelian Higgs model, the plaquette quantum numbers are the dual variables. If we impose periodic boundary conditions on the plaquettes, we can only have neutral states. This is a manifestation of Gauss' s law. We can however probe the charged sector by introducing a Polyakov loop, a Wilson loop wrapping around the imaginary time dimension and the order parameter for deconfinement. For a more sophisticated treatment of related questions in QED see ref. [16].

The Tensor Renormalization Group (TRG) code for the two-dimensional Abelian Higgs model was formulated in terms of the gauge interaction plaquette quantum numbers which are the dual variables to a two-dimensional lattice spin model. Calculating the free energy using TRG is simple, and from that, typical thermodynamic quantities can be calculated immediately. The Monte Carlo (MC) code for the Abelian-Higgs model, as well as the TRG code, were cross checked with each other using first and second derivatives of the free energy, as well as the expectation value of the Polyakov loop. Good agreement was found in all cases (all values agreed within error bars) between MC and TRG using only a moderate number of states, across a wide range of κ and β values (across approximately two magnitudes of ten).

For the measurement of the Polyakov loop, it is necessary to locally tune a term in the Hamiltonian for a particular site of the optical lattice. We propose this as a useful way to probe the deconfinement transition. Even though the experimental set-up and measurement for this quantity is quite challenging, there has been rapid experimental progress on single-site-resolved control and measurement in cold atom experiments [18, 21, 22].

(4) Education and training.

This project supported training of two graduate students, Dr. Chen-Yen Lai (PhD 2014) and Mr. Jin Zhang, and one postdoctoral researcher, Dr. Alexei Bazavov.

Two high school students (Mr. Jens Dancer and Ms. Sonali Durham, from Iowa City High School, Iowa City, IA) and two undergraduate students (Mr. Keshav Suttrave and Mr. Zhuohao Liu, from University of Iowa) were mentored during this reporting period, with support from the HSAP/URAP program for two of them. In their projects, the students studied concepts of quantum physics and statistical mechanics, made calculations for the Ising model and related clock models, learned computer coding, participated in group meetings, gave presentations and wrote a final report. The project was led by Prof. Yannick Meurice. The students also interacted closely with Dr. Alexei Bazavov and graduate students from University of Iowa, and participated in conference calls with the University of California Riverside side of this project.

The University of California Riverside is a 2003 U.S. Department of Education Accredited Postsecondary Minority Institution pursuant to the Higher Education Act (20 U.S.C. Section 1067k(3)) and its student population reflects the diversity of its community. Prof. Shan-Wen Tsai, participated in the Summer Physics Academy for high-school teachers, hosted by the Department of Physics and Astronomy of the University of California Riverside [23], with a refresher course on "Thermal Physics" that included various demonstrations and hands-on activities. During the discussion on the concept of temperature, she also briefly discussed research on the frontiers of ultra-cold atoms and the prospects of quantum simulating models studied in Condensed Matter Physics and Lattice Gauge Theory. The goal of this Summer Academy is to reach out to local high-school students (and future college students) through their teachers, and to encourage them to learn physics and be prepared for physics courses at the college level.

(5) Bibliography

[1] H. Zou, Y. Liu, C.-Y. Lai, J. Unmuth-Yockey, L.-P. Yang, A. Bazavov, Z. Y. Xie, T. Xiang, S. Chandrasekharan, S.-W. Tsai, and Y. Meurice, "Progress towards quantum simulating the classical $O(2)$ model", *Physical Review A* 90, 063603 (2014).

[2] A. Bazavov, Y. Meurice, S.-W. Tsai, J. Unmuth-Yockey, and J. Zhang, "Gauge-invariant implementation of the Abelian Higgs model on optical lattices", *Physical Review D* 92, 076003 (2015).

[3] A. Bazavov, C.-Y. Lai, S.-W. Tsai, and Y. Meurice, "The effective $U(1)$ -Higgs theory at strong coupling on optical lattices?",

Proceedings for the XXXII International Symposium on Lattice Field Theory, June 23-28, 2014, Columbia University, New York City, NY (2014).

[4] A. Bazavov, Y. Meurice, S.-W. Tsai, J. Unmuth-Yockey, J. Zhang, “Effective action for the Abelian-Higgs model for a gauge-invariant implementation on optical lattices”, Proceedings for the XXXIII International Symposium on Lattice Field Theory, July 14-18, 2015, Kobe, Japan (2015).

[5] L.-P. Yang, Y. Liu, H. Zou, Z. X. Xie, and Y. Meurice, “The fine structure of the entanglement entropy in the classical XY model”, Physical Review E 93, 012138 (2016).

[6] Y. Meurice, L.-P. Yang, J. Unmuth-Yockey, Y. Liu, J. Osborn, Z. Xie, H. Zou, “Approaching conformality with the Tensor Renormalization Group method”, Proceedings for the XXXIII International Symposium on Lattice Field Theory, July 14-18, 2015, Kobe, Japan (2015).

[7] Yuzhi Liu, Y. Meurice, M. P. Qin, J. Unmuth-Yockey, T. Xiang, Z. Y. Xie, J. F. Yu, and H. Zou, “Exact blocking formulas for spin and gauge models”, Physical Review D 88, 056005 (2013) and references therein.

[8] Y. Meurice, “Accurate exponents from approximate tensor renormalizations”, Physical Review B 87, 064422 (2013).

[9] A. Denbleyker, Yuzhi Liu, Y. Meurice, M. P. Qin, J. Unmuth-Yockey, T. Xiang, Z. Y. Xie, J. F. Yu, and H. Zou, “Controlling sign problems in spin models using tensor renormalization”, Physical Review D 89, 016008 (2014).

[10] <http://www.scidac.gov>

[11] usqcd.fnal.gov/software.html

[12] J. Heitger, “Numerical simulations of Gauge-Higgs models on the lattice”, PhD. Thesis (1997).

[13] B. Bunk, “Monte Carlo methods and results for the electro-weak phase transition”, Nucl. Phys. Proc. Suppl. 42, 566 (1995).

[14] A. Bazavov and B. A. Berg, “Heat bath efficiency with metropolis-type updating”, Phys. Rev. D 71, 114506 (2005).

[15] <http://www.usqcd.org>

[16] C.-Y. Lai, W.-M. Huang, D. K. Campbell, and S.-W. Tsai, “dxy-density wave in fermion-fermion cold-atom mixtures”, Physical Review A 90, 013610 (2014).

[17] P. Calabrese and J. L. Cardy, “Entanglement entropy and quantum field theory”, Journal of Statistical Mechanics: Theory and Experiment 0406, P06002 (2004).

[18] R. Islam, R. Ma, P. M. Preiss, M. E. Tai, A. Lukin, M. Rispoli, and M. Greiner, “Measuring entanglement entropy in a quantum many-body system”, Nature 528, 77 (2015).

[19] K.-A. B. Soderberg, N. Gemelke and C. Chin, “Ultracold molecules: vehicles to scalable quantum information processing”, New Journal of Physics 11, 055022 (2009).

[20] B. Lucini, A. Patella, A. Ramos, and N. Tantalo, “Charged hadrons in local finite-volume QED+QCD with C_4 boundary conditions”, Journal of High Energy Physics 2, 76 (2016).

[21] J. H. Lee, E. Montano, I. H. Deutsch, and P. S. Jessen, “Robust site-resolvable quantum gates in an optical lattice via inhomogeneous control”, Nature Communications 4, 3027 (2013).

[22] T. Fukuhara, S. Hild, J. Zeiher, P. Schauss, I. Bloch, M. Endres, and C. Gross, “Spatially Resolved Detection of a Spin-Entanglement Wave in a Bose-Hubbard Chain”, Physical Review Letters 115, 035302 (2015).

[23] “RIVERSIDE: UCR academy hosts high school physics teachers”, The Press Enterprise, July 28, 2015 (<http://www.pe.com/articles/physics-774975-teachers-academy.html>).

Technology Transfer